IMPACT OF INSERTION REACTION OF $O(^1D)$ INTO THE CARBONIC ACID MOLECULE IN THE ATMOSPHERE OF EARTH AND MARS

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In this talk, we present the energetics and kinetics of the insertion reaction of the $O(^1D)$ into the H_2CO_3 molecule that finally produces the percarbonic acid $[H_2C(O)O_3]$ molecule $(H_2CO_3 + O(^1D) \rightarrow H_2C(O)O_3)$. The rate constants have been calculated by the Variable-Reaction-Coordinate Variational Transition State Theory $(VRC-VTST)$. From our results, we show that the rate constants of the insertion reaction are significantly higher than the rate constants associated with the H_2O-assisted H_2CO_3 decomposition $(H_2CO_3 + H_2O \rightarrow CO_2 + 2H_2O)$, acetic acid (AA)-assisted H_2CO_3 decomposition $(H_2CO_3 + AA \rightarrow CO_2 + H_2O + AA)$ and OH radical-initiated H_2CO_3 degradation reaction $(H_2CO_3 + OH^{\cdot} \rightarrow HCO_3 + H_2O)$ −which are currently assumed to be the potentially important reaction channels to interpret the atmospheric loss of the H_2CO_3 molecule in the Earth. Finally, we also discuss the potential impact of the H_2O-assisted H_2CO_3 decomposition reaction, OH radical-initiated H_2CO_3 degradation reaction and the above-mentioned insertion reaction on equal footing toward the loss of H_2CO_3 molecule, especially, in the surface of Mars.

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